

4-Phenyl-4h-1,3,4-thiadiazine-2(3h)-thione

Inchi:	InChI=1S/C9H8N2S2/c12-9-10-11(6-7-13-9)8-4-2-1-3-5-8/h1-7H,(H,10,12)
InchiKey:	PXSYTNKEAVUXCF-UHFFFAOYSA-N
Formula:	C9H8N2S2
SMILES:	S=C1NN(c2ccccc2)C=CS1
Mol. weight [g/mol]:	208.30
CAS:	17374-23-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	2.500		Crippen Method
mcvol	147.110	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17374231&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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